

Robust optical conductivity in gapped graphene

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We study the optical conductivity in the low-energy regime of gapped mono- and bilayer graphene. A scaling relation is found, in which the four parameters frequency, gap, Fermi energy and temperature appear only as combination of three independent parameters. The ratio of the optical conductivity of bilayer and monolayer graphene is exactly 2.

I. INTRODUCTION

Monolayer and bilayer graphene are semimetals with good conducting properties [1–3]. Moreover, in the presence of a microwave field the related optical conductivity is constant over a large regime of frequencies. This has been found in theoretical calculations [4–8] and was also observed experimentally [9, 10]. The reason for this behavior is the existence of at least two bands in both materials, where at Fermi energy $E_F = 0$ (i.e. graphene without a gate potential) the lower band is occupied and the upper band is unoccupied. As consequence, the absorption of photons of energy $\hbar\omega$ from the microwave field creates electron-holes pairs due to the excitation of electrons from the lower band at energy $-\hbar\omega/2$ to the unoccupied upper band at energy $\hbar\omega/2$. This mechanism applies also to gated graphene which has a shifted Fermi energy $E_F \neq 0$. However, in this case photons can only be absorbed if $\hbar\omega/2 > E_F$ (for $E_F > 0$), since all the states in the upper band are occupied up to the energy E_F . Correspondingly, a photon can only be absorbed for $-\hbar\omega/2 < E_F$ if $E_F < 0$. This means that electron-hole creation by a microwave field is only possible if $\hbar\omega > |E_F|$.

It has been found in a number of recent experiments that the creation of a gap in the semimetallic band structure of monolayer graphene (MLG) is possible by absorption of hydrogen [11] or in bilayer graphene (BLG) by applying a double gate [12]. In both cases an electron-holes pair can also be created but this requires a photon energy larger than the band gap Δ (cf. Fig. 1).

Once electron-holes pairs have been created they will contribute to a current in the material, where the latter is related to the strength of the external microwave field by the optical conductivity $\sigma_{\mu\mu}(\omega)$. This quantity can be measured experimentally and characterizes the electronic properties of the material. In particular, it can be used to determine the band gap Δ , since it vanishes for $\hbar\omega \leq \Delta$. BLG, in contrast to MLG, has two low- and two high-energy bands. As a result, there are several gaps that lead to electron-hole pair creations on different energy scales with a more complex behavior of the optical conductivity [13–15].

In the following the optical conductivity shall be evaluated via the Kubo formalism for the low-energy bands in MLG and BLG at nonzero temperature T . This avoids electron-hole pair creation from higher energy bands and van Hove singularities. An important question in this context is the role of the low-energy quasiparticle spectrum on the optical conductivity. In order to focus on simple spectral properties, we consider only non-interacting electrons in a periodic tight-binding model. Thus disorder, electron-electron interaction and electron-phonon interaction are not taken into account.

II. MODEL CALCULATION

The low-energy quasiparticle states in MLG with a gap $\Delta = 2m$ are described by the massive two-dimensional Dirac equation

$$\mathbf{H}_M \begin{pmatrix} \Psi_\uparrow \\ \Psi_\downarrow \end{pmatrix} = \begin{pmatrix} -E + m & i\partial_x + \partial_y \\ i\partial_x - \partial_y & -E - m \end{pmatrix} \begin{pmatrix} \Psi_\uparrow \\ \Psi_\downarrow \end{pmatrix} = 0. \quad (1)$$

For simplicity, we have set the Fermi velocity $v_F = 1$ because this parameter will not appear in the final results for the conductivity. A similar equation exists for the low-energy quasiparticle states of BLG

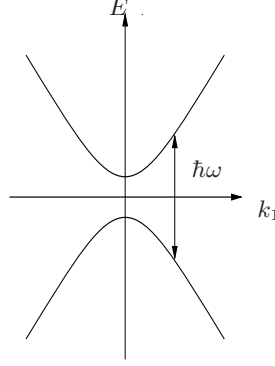


FIG. 1: Schematic picture of the creation of an electron-hole pair in gapped mono- or bilayer graphene by the absorption of a photon with energy $\hbar\omega$. For this process the photon energy must be larger than the band gap $\Delta = 2m$.

[16, 17]:

$$\mathbf{H}_B \begin{pmatrix} \Psi_{\uparrow} \\ \Psi_{\downarrow} \end{pmatrix} = \begin{pmatrix} -E + m & (i\partial_x + \partial_y)^2 \\ (i\partial_x - \partial_y)^2 & -E - m \end{pmatrix} \begin{pmatrix} \Psi_{\uparrow} \\ \Psi_{\downarrow} \end{pmatrix} = 0. \quad (2)$$

With the plane-wave ansatz $\Psi_{\downarrow}(x, y) = \Psi_{\downarrow} e^{ik_x x + ik_y y}$ we obtain for MLG the following relations

$$\Psi_{\downarrow}(x, y) = \frac{k_x + ik_y}{E + m} \Psi_{\uparrow}(x, y), \quad E^2 = m^2 + k^2 \quad (3)$$

and for BLG

$$\Psi_{\downarrow}(x, y) = \frac{(k_x + ik_y)^2}{m + E} \Psi_{\uparrow}(x, y), \quad E^2 = m^2 + k^4. \quad (4)$$

These solutions will be used as a basis for evaluating current matrix elements and the optical conductivity.

Kubo formula: The optical conductivity can be calculated from the Kubo formula. This requires the evaluation of the current operator $j_{\mu} = ie[\mathbf{H}, r_{\mu}]$, where r_{μ} ($\mu = 1, 2$) is a component of the position of the quasiparticle. The nonzero matrix elements of the current operator with respect to the energy eigenstates of Eqs. (3), (4) are either diagonal elements $ie\langle E_k | [H, r_{\mu}] | E_k \rangle$ or the off-diagonal elements $ie\langle E_k | [H, r_{\mu}] | -E_k \rangle$. It turns out that the diagonal elements do not appear in the real part of the optical conductivity [18]. Only the off-diagonal terms contribute because the optical conductivity requires a scattering process between two states whose energy difference is just the photon energy ω . A convenient representation of the Kubo formula then is [18]

$$\sigma'_{\mu\mu} \equiv \text{Re}(\sigma_{\mu\mu}) = \frac{\pi e^2}{4\hbar} \int |\langle E_k | [H, r_{\mu}] | -E_k \rangle|^2 \delta(E_k + \omega/2) \frac{f_{\beta}(E_F - E_k) - f_{\beta}(E_F + E_k)}{E_k} \frac{d^2 k}{(2\pi)^2}$$

with the Dirac-Fermi distribution $f_{\beta}(x) = 1/(1 + e^{\beta x})$ at inverse temperature $\beta = 1/k_B T$. (Here and in the rest of this paper the spin and valley degeneracy, providing an extra factor 4, has not been written explicitly.) Integration over E_k gives

$$\sigma'_{\mu\mu} = -\frac{e^2}{4\hbar} \int_0^{2\pi} |\langle \omega/2 | [H, r_{\mu}] | -\omega/2 \rangle|^2 d\varphi J \frac{f_{\beta}(E_F + \omega/2) - f_{\beta}(E_F - \omega/2)}{\omega} \quad (5)$$

with the Jacobian J from the radial k integration:

$$J = \Theta(\omega^2 - m^2/4) \begin{cases} \omega/2 & \text{MLG} \\ \omega/2\sqrt{\omega^2 - 4m^2} & \text{BLG} \end{cases}.$$

current matrix elements: The commutator in the current operator is for Dirac fermions the Pauli matrix σ_μ : $[\mathbf{H}_M, r_\mu] = i\sigma_\mu$ (MLG) and for BLG in Fourier representation

$$[\mathbf{H}_B, x] = i \frac{\partial \mathbf{H}_B}{\partial k_x} = 2i(k_x \sigma_1 + k_y \sigma_2) .$$

Then for the current matrix element for MLG we obtain

$$|\langle E | \sigma_1 | -E \rangle|^2 = \frac{m^2 + k_y^2}{E^2} \quad (6)$$

which after angular integration yields

$$\int_0^{2\pi} |\langle E | \sigma_1 | -E \rangle|^2 d\varphi = \pi \frac{2m^2 + k^2}{E^2} = \pi \frac{m^2 + E^2}{E^2} . \quad (7)$$

For BLG (with $k^2 = \sqrt{\omega^2/4 - m^2}$, $k_x = k \cos \varphi$ and $k_y = k \sin \varphi$) we have

$$|\langle E | k_x \sigma_1 + k_y \sigma_2 | -E \rangle|^2 = k^2 \left[\frac{m^2}{E^2} + 4 \frac{k^4}{E^2} (\cos^2 \varphi - \sin^2 \varphi) \cos^2 \varphi \sin^2 \varphi + \frac{k^4}{E^2} \sin^2 \varphi + \frac{2m}{E} \cos \varphi \sin \varphi \right] \quad (8)$$

and after the angular integration

$$\int_0^{2\pi} |\langle E | k_x \sigma_1 + k_y \sigma_2 | -E \rangle|^2 d\varphi = \pi k^2 \frac{m^2 + E^2}{E^2} . \quad (9)$$

This is valid only for $\omega^2 \geq 4m^2 = \Delta^2$. As an example, these current matrix elements are plotted for $E = 2$ in Fig. 2 with and without gap.

conductivity: Now we insert the results of Eq. (7) into the Kubo formula Eq. (5) and obtain for MLG

$$\sigma'_{MLG} = \frac{\pi e^2}{8h} \left[1 + \frac{\Delta^2}{\omega^2} \right] \Theta(\omega^2 - \Delta^2) [f_\beta(E_F + \omega/2) - f_\beta(E_F - \omega/2)] . \quad (10)$$

Inserting Eq. (9) into the Kubo formula gives exactly twice the conductivity of MLG: $\sigma'_{BLG} = 2\sigma'_{MLG}$. Thus the conductivities of MLG and BLG agree up to a factor 2. The additive correction due to the gap parameter Δ^2 decays like ω^{-2} . As an example, the behavior of the conductivity versus $\omega/k_B T$ is plotted in Fig. 3.

III. DISCUSSION

The conductivity in Eq. (10) obeys a scaling relation of the conductivity:

$$\sigma'_{xx}(\beta, \Delta, E_F, \omega) = \sigma'_{xx}(\beta\Delta, \beta E_F, \beta\omega) = \sigma'_{xx}(\Delta/\omega, \beta E_F, \beta\omega) ,$$

i.e. the conductivity depends only on three independent parameters. A similar scaling relation exists also for the conductivity in the presence of a scattering rate [5]. This implies that a reduction of temperature is equivalent to a simultaneous increase of frequency, gap and Fermi energy.

The optical conductivity vanishes for photon energies less than the gap. It jumps to some finite value when the photon energy exceeds the gap energy, where the size of the jump depends on the Fermi energy (cf. Fig. 3). The maximal jump appears at $E_F = 0$. This allows us to measure the gap by measuring the jump of the optical conductivity. Such a measurement can be performed as an optical transmission experiment [9, 19] because the optical conductivity is related to the transmittance T through the relation

$$T = \frac{1}{1 + 2\pi\sigma'_{xx}/c} .$$

The parameter c is the speed of light. Then graphene is completely transparent for photonic energies up to the gap energy. This could be used to filter light with frequencies higher than the one given by the gap energy.

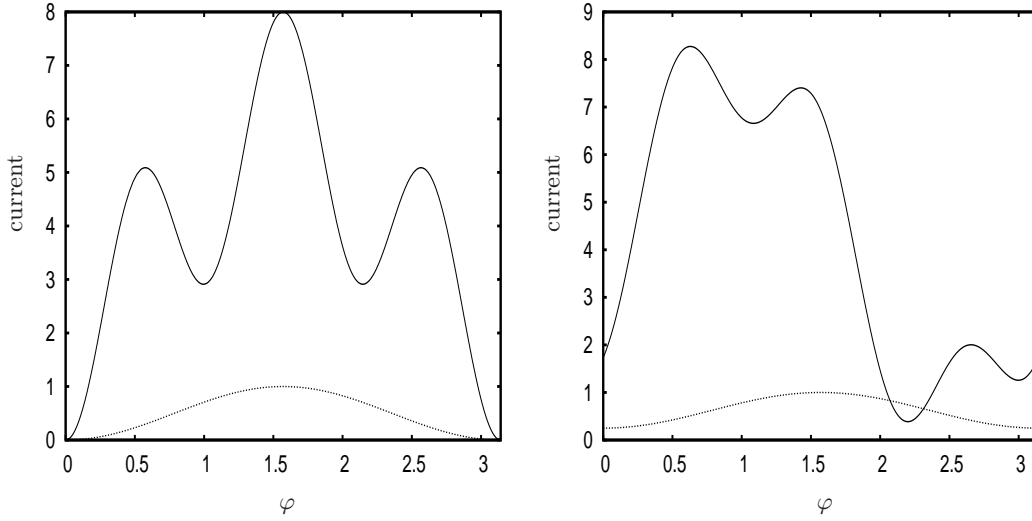


FIG. 2: The current matrix element $|\langle E | [\mathbf{H}, x] | - E \rangle|^2$ as a function of the angle φ between the wave vector \mathbf{k} and the direction of the current operator. The left panel is the matrix element for $E = 2$ without gap ($m = 0$) and the right panel is the matrix element with gap ($\Delta = 2m = 2$). Full (dashed) curves are for BLG (MLG).

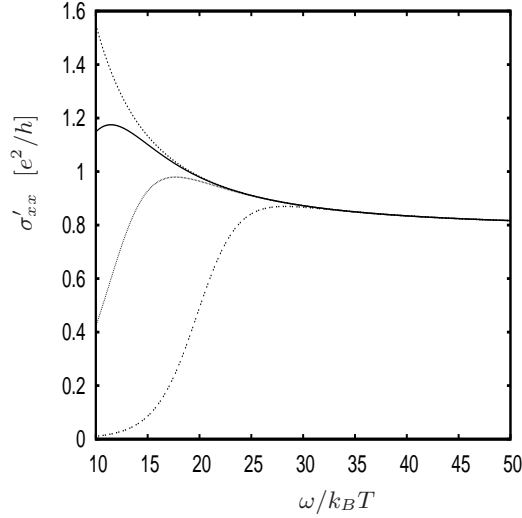


FIG. 3: Optical conductivity of BLG as a function of $\beta\omega$ for $\beta m = 5$ and $\beta E_F = 0, 4, 6, 10$ with decreasing conductivity. These curves have to be multiplied by $1/2$ to get the corresponding values for MLG.

Our model assumption of taking into account only the low-energy bands of BLG restricts the photon energies $\hbar\omega$ to less than 0.8eV, which is the gap between the low-energy and the high-energy bands in BLG [13, 14]. This restriction also avoids stronger deviations from the Dirac theory of MLG and van Hove singularities. Taking into account high-energy bands does not change this picture qualitatively, since it would lead to additional jumps of the optical conductivities as soon as the photon energies exceed the gap energies. A van Hove singularity would appear as an additional peak. The effect of the gap is a global enhancement by m^2 , where for BLG the situation is more complex than for MLG.

In conclusion, focusing on the low-energy dispersion of gapped monolayer and bilayer graphene, we have found simple expressions for the optical conductivities. They agree for all parameters up to a factor 2. This is remarkable because the current-matrix elements of both graphene systems are rather different.

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